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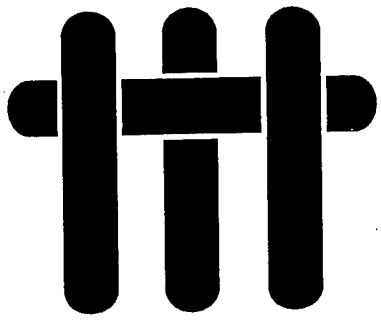

A KNOWLEDGE HIGHWAY FOR INTEGRATED MODELLING FROM MANUFACTURING TO DESIGN

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A workshop was held to discuss a new paradigm for choosing the preferred materials and processes needed for manufacturing a component, based on an analysis of the targeted attributes, performance and cost. This paradigm was developed around the idea of a "knowledge highway"--a disciplined process for generating, storing and using the information most relevant to the manufacturing and design engineers. Model systems were used to develop this idea, which combined many of the technical aspects of greatest concern in manufacturing and design--processing, microstructural evolution, property profiles, fail-safe design, and costing. The concept integrated experimental studies, simulation and analysis. The final result would be software designed to be used by manufacturing and design engineers in selecting materials and processes to meet specific technical/commercial objectives.

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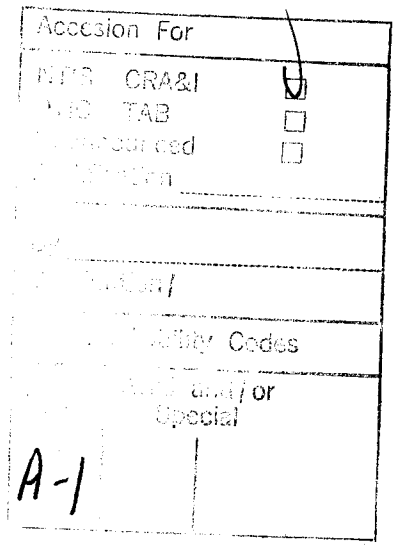


1. SYNOPSIS

This initiative combines research groups from University, Industry and National Laboratories in order to develop a new paradigm for choosing the preferred materials and processes needed for manufacturing a component, based on an analysis of the targeted attributes, performance and cost. This paradigm will be developed around the idea of a "knowledge highway"—a disciplined process for generating, storing and using the information most relevant to the manufacturing and design engineers. Model systems will be used to develop this idea, which combine many of the technical aspects of greatest concern in manufacturing and design—processing, microstructural evolution, property profiles, fail-safe design, and costing. The project would integrate experimental studies, simulation and analysis. The final result will be software designed to be used by manufacturing and design engineers in selecting materials and processes to meet specific technical/commercial objectives.

The actual implementation of concurrent engineering (CE) concepts in both industry and academia has been quite limited in scope. Manufacturing engineers do not routinely communicate with design and product engineers. One of the difficulties has been the lack of a methodology, with common engineering terminology, that permits such communication to occur. Moreover, usage of the CE concept could become widespread if a hierarchy of models exists that connect the parameters used in manufacturing to the material properties used for product design and lifing. Ideally, industry would wish to have a capability for simulating the manufacturing process in a manner that leads directly into a code for predicting product performance (Fig. 1.1). Stated simply, the product engineer could systematically explore all of the materials potentially usable for a product, along with their processing options, by using a methodology that simulates the process, the microstructure and the defects, and then use output to calculate the material properties and the product performance. Moreover, integration with cost models would allow life cycle costs to be estimated and used to differentiate materials and processes on the basis of cost, as well as performance. For example, a hot section turbine vane in a propulsion unit could be made from a superalloy, a ceramic-coated superalloy, a monolithic ceramic, a metal matrix composite or a ceramic matrix composite. Each of these materials has several manufacturing options. The superalloy could be formed by investment casting, by hot forging (followed by machining) or by hot isostatic pressing from powder. Each material and processing method has associated costs and produces a component having specific physical and chemical property profiles. A modeling methodology for predicting which material and which process should result in a vane that satisfies the system performance goals with acceptable life-cycle costs would have

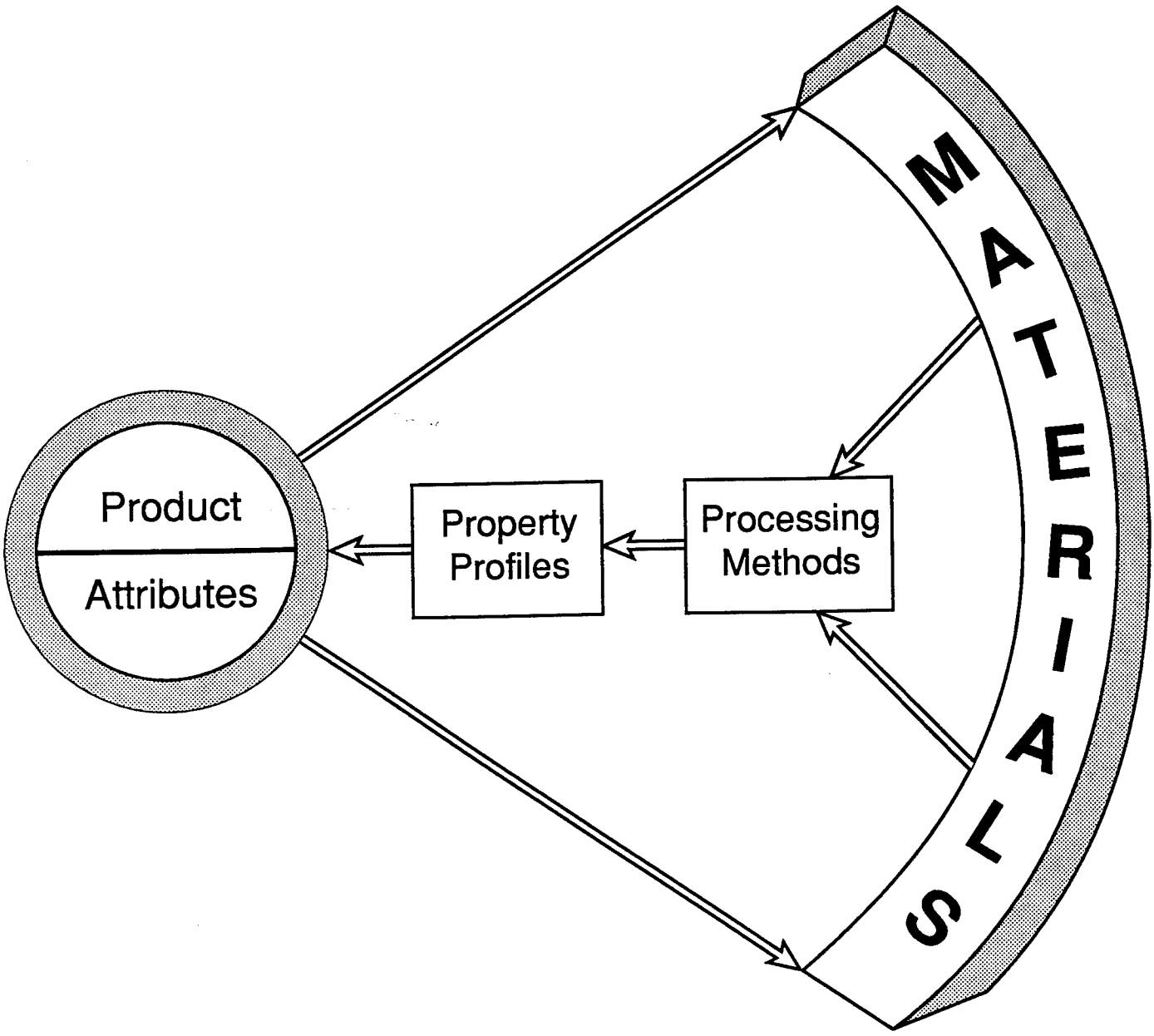

MATERIALS
Product
Attributes
Property
Profiles
Processing
Methods

Figure 1.1

a major influence on the design engineer's ability to make decisions that substantially reduce the time and cost between conceptual design and implementation.

While the realization of this objective has many difficult challenges, it is judged that the development of the core discipline is a tractable problem that could be put in place through a collaborative activity involving engineers from academia, industry and government laboratories. The basic concept (Fig. 1.2) is the creation of a Knowledge Highway. The Highway would be in the form of a framework that links together models that range from processing to performance, with microstructure and defect models as the connecting entities.

The models to be incorporated into the Knowledge Highway might not initially be mechanism-based. Instead, some might be analytical, but with numerical coefficients to be obtained through selected experiments. Others might be empirical. A good example of the concept is illustrated in the modelling integration used to relate processing to performance for components made from precipitation-hardened Al alloys [1]. The Highway would also embrace codes that either exist now or would soon be developed, which comprehensively address some of the requirements. These could include fluid flow and heat transfer codes, such as Physica, and software for atomistic calculations, available through BIOSYM, etc.

The integration of cost models with engineering models is considered to be an additional important objective. These would be life cycle models that incorporate engineering principles into parameters used for global, (bottom-down) cost models, such as capital and material costs, as well as various time-dependent factors. Such global models are in demand by industry and would not conflict with the local level modelling presently used within the industrial domain.

The development of a Knowledge Highway and the testing of its utility can only be achieved by having a focus on specific products. Several examples have been briefly considered as candidates for comprehensive investigation. These are discussed and conclusions made about the potential for successfully accomplishing the objectives.

Various terminologies are used throughout this report which may require clarification. The definitions are given in table I.

The output of the research would be modular backbone code that allows specific process models, performance models, etc., to be introduced by the user. It would recommend model options that identify data requirements and indicate situations requiring experimental information to either

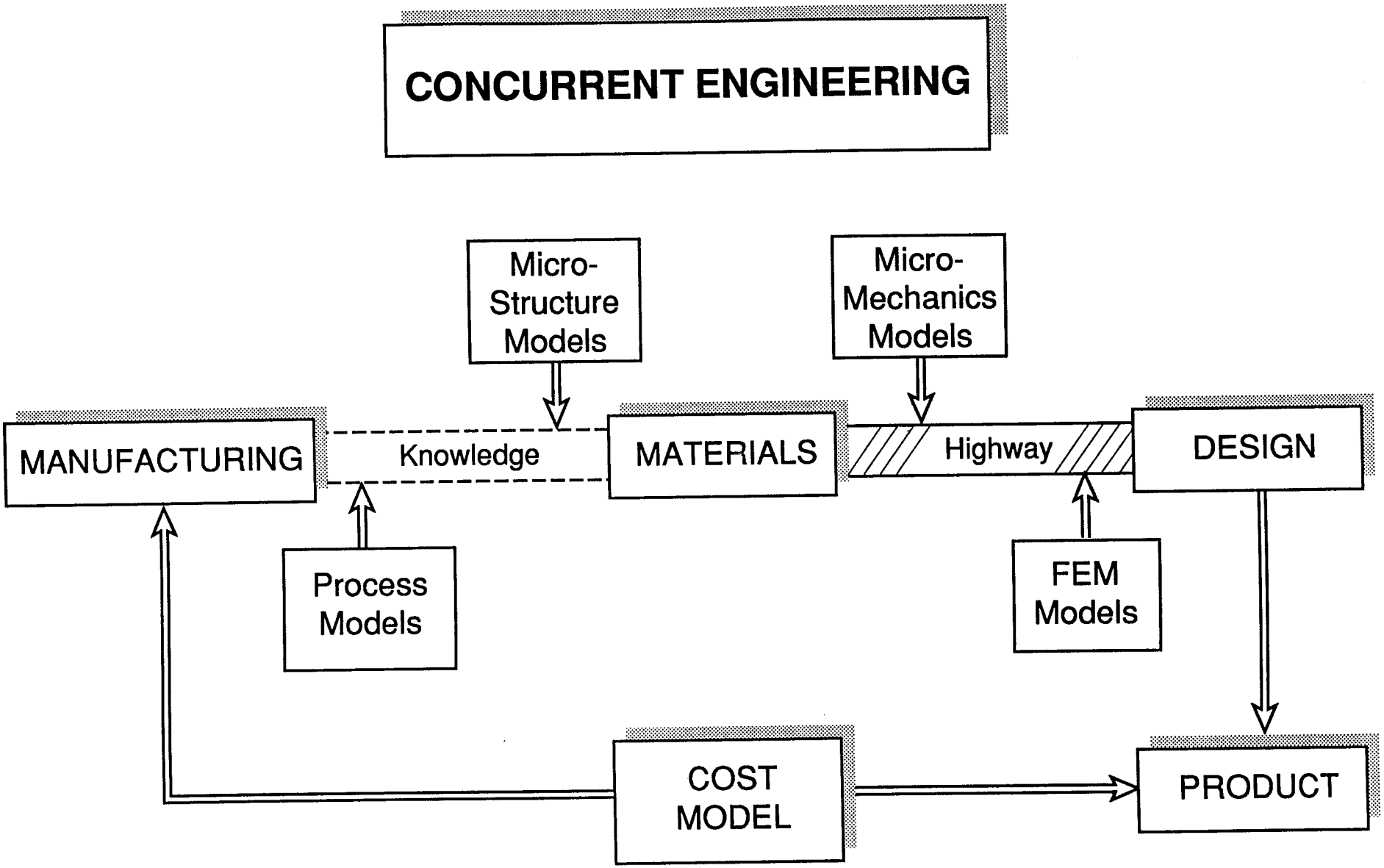

CONCURRENT ENGINEERING
Micro-
Structure
Models
Micro-
Mechanics
Models
MANUFACTURING
Knowledge
MATERIALS
Highway
DESIGN
Process
Models
FEM
Models
COST
MODEL
PRODUCT

Figure 1.2

calibrate or make linkages between models. Experimental methods, test protocols and data analysis would be recommended. The final program would be made available through collaborations with a professional software company.

TABLE I
Definitions

Product:	A component that has a critical influence on system performance, yield, reliability and cost. An example would be a coated turbine blade in a propulsion system.
Product Attributes:	Each product has specific attributes governed by its function in the system. The design engineer has an attribute set that governs the design process. For example, a coated turbine blade must withstand a temperature and rotational speed profile for a specific number of cycles without experiencing any failure modes, such as excessive creep distortion, fatigue failure, catastrophic oxidation, coating spallation. Moreover, it must achieve stringent manufacturing and other cost goals. To attain these attributes, the material must satisfy a physical and chemical property profile and be amenable to inherently reproducible processing into the design configuration.
Process Models:	These are models that predict various macroscopic characteristics of a finished product made by a particular process. For example, an optimized process model for casting would predict temperature distributions throughout the mold and within the solidifying body in terms of the boundary conditions imposed through the control system. It would also predict the flow field in the liquid and the mushy zone caused by temperature and concentration gradients. It would then predict the rate of solidification and the composition gradients in the solid.
Microstructure Models:	These are models that use the temperature, stress, flow field information generated in the process model and predict the microstructure expected in the final body. The features to be predicted include grain size, porosity, solute segregation, etc.
Performance Models:	These are preferably mechanism-based models that begin with the microstructure and predict various physical properties such as yield strength, fracture toughness, creep strength, fatigue threshold, etc.

2. CONSIDERATIONS FOR SUCCESSFUL MODELLING

2.1 Criteria

Before embarking on a major modelling exercise, experience has demonstrated that the following conditions should be met.

1. Underlying Physics. The underlying physics of each step in the process (that is, each individual mechanism involved) must be understood. The timescale for developing new physical understanding is uncertain. An example of not yet understood physics is the mechanism of laser-plasma interaction.

2. Coherent Modelling Plan. In a flow chart comprising the modules for the overall model, it must be established that resources exist to implement each: (experience, expertise, hardware, software tools, and understanding), and also that their interfaces present no insurmountable problems. One missing link could jeopardize the entire model. For this reason, the model should be structured in separable modules. Initially some of these can be purely empirical (simply a curve fit describing some aspect of the behavior) when more sophisticated models prove elusive. As understanding increases, those can be replaced by physics-based models. A key ingredient is a structure which allows this evolution in modelling sophistication. Ideally, the model should function at any moment during its development: initially at a very crude level; finally at a more sophisticated level. In this way, its overall functioning can be tested continuously.

3. Value added (or scale) in the process. The value added to the product by the real process must either be large, or its throughput considerable, to justify a large-scale modelling activity. The revenue generated by the improvements brought about by the model must at least pay for the model itself. It is not always obvious that this will be the case. But, choosing processes with very high added value and with an established market, ensures that this criterion is satisfied.

4. Timescale. If "intelligent" real-time, model-based control of a process is envisaged, then it must be possible to permit sensing, running of the model, and the implementation of its outputs to change the process conditions all in a timescale that is short compared with that of the process itself. Thus slow deposition processes (like PVD) or consolidation processes (like HIPing) lend themselves well to model-based real-time control.

2.2 Modelling Tools

1. Hierarchy of Structural Scales

It is widely appreciated that material behavior involves several structural scales from atomistic to continuum (Fig. 2.1). Within each structural level, methods have evolved to describe and characterize the structure, and, often, its evolution. Linking one scale level to the next is the challenge. To do this, *filters* or *gates* are needed. The information developed at one level is seldom in the form required as the input to the next level up. For example, the enormous detail known about the behavior of single dislocations provides minimal help in describing the micromechanics of plasticity, in which large numbers of dislocations are involved. A focus on these interfaces is especially important.

There is another interesting concept. Failure at one level is "damage" at the next level up. A critical level of damage at the next level up causes failure at that level, and damage at the next. As an example: one broken atomic bond does not cause the sample to fail. But enough broken bonds, aggregated into a critical crack, cause failure of the component. The structure built from such components will not necessarily fail, but it is now damaged. As an example, a strut in a redundant structure, having failed, does not cause failure of the structure, although it is now weaker. Several failed struts could cause failure of the structure itself. Concepts of this sort, which rely on interscale relationships, are in need of development.

2. Post Processing of Simulations

Simulations give too much information. Tools are needed that help extract the key results which can then be captured in simpler framework, similar to the filters or gates in the structural hierarchy.

3. Mechanism Maps

Maps give an overview of "modelling space". The axes are the key modelling parameters or dimensionless groups. They show the fields within this space in which given mechanisms or modes of behavior are dominant. The utility of the maps lies here. Once an area of the space is identified as important in a practical problem, the map identifies the mechanism of importance, and thus the modelling module relevant to that problem. Maps, till now, have had only limited impact because this last stage has not been successfully implemented.

Innovative Material Design

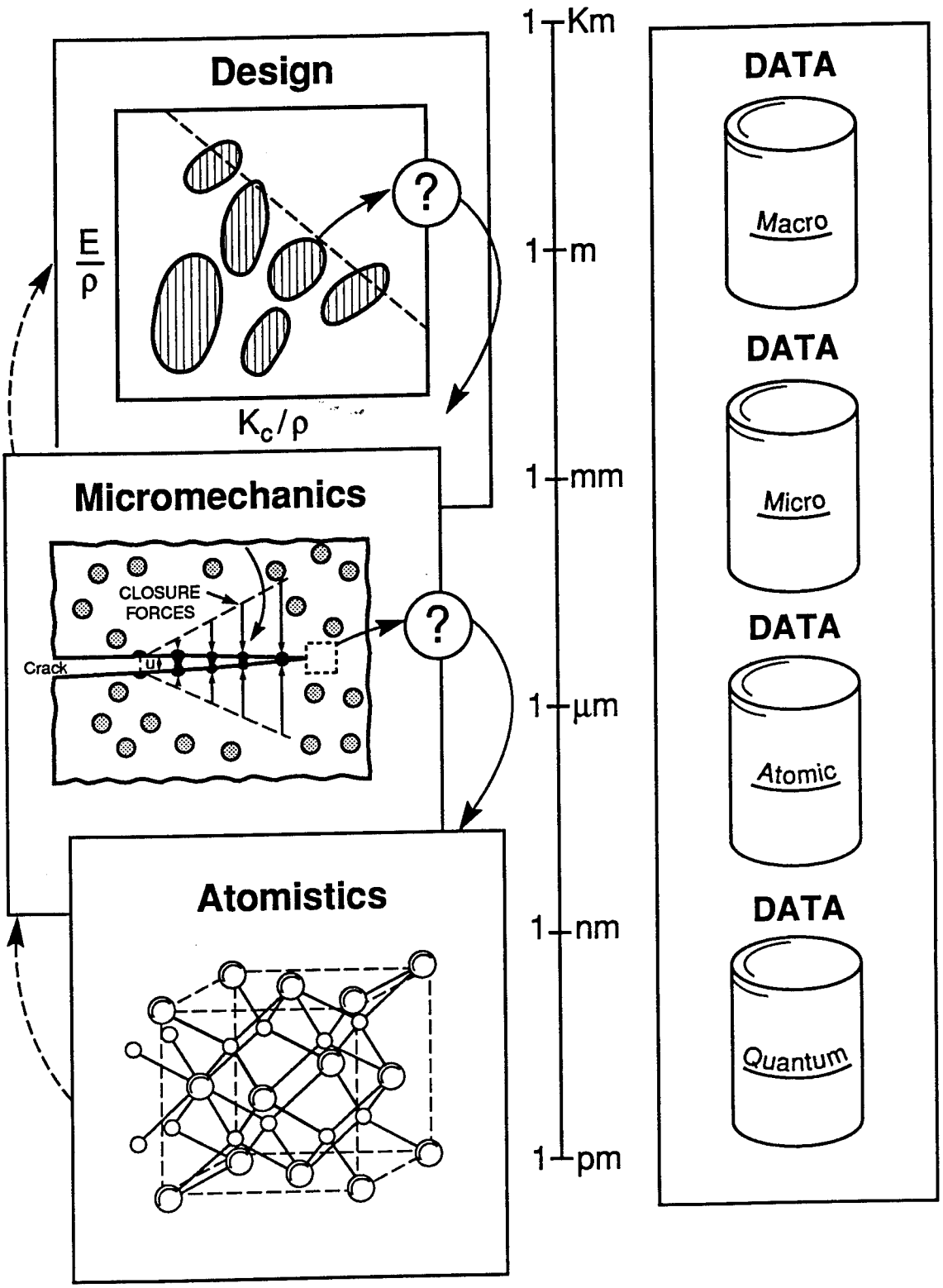


Figure 2.1

3. THE LIFE CYCLE CONCEPT

To achieve an integrated methodology, the models devised for process analysis and for cost estimation, as well as those used for predicting property profiles, must be formulated using common variables which describe the current state of the material. However, the important state variables are product dependent. The product attributes are often experience-based measures of performance, which are not usually related in an explicit way to well-defined combinations of thermophysical properties. For example, in automobile panels, the resistance to *deflection* and *distortion* at minimum weight when subject to localized forces is an important *attribute*. In this simple case, design formulae provide merit indices based on modulus, E, density, ρ, and yield strength, σ_y. Therefore, the state variables which carry through the process models must have compositional and microstructural information that can be related to E, ρ and σ_y.

Product *life* represents another essential *attribute*. The limiting mechanisms are typically fatigue, corrosion and wear/erosion. In the case of fatigue, porosity is often an important variable because of its effect on crack initiation and low cycle fatigue. A key objective of a process model relevant to a fatigue limited product is the simulation of porosity evolution during sequential steps in the processing. Yet, most process models do not include porosity as a variable. Existing process models attempt to simulate grain evolution and (in some cases) precipitation. These variables may be used to predict yield and creep strength, but may be incidental to fatigue life.

A simple example is presented in order to illustrate the concept. The model employs evolving physicoeconomic states to design a product for minimum cost over any desired portion of the product life cycle. The approach is exemplified by a truck wheel, modelled as a simple disc forged from a cylindrical aluminum alloy casting. The physicoeconomic state is assumed to be described by five parameters: alloy content, a; diameter, d; thickness, h; strength, s; and cost, c. The design is based upon the entire life cycle, including costs of initial casting, manufacture, use and disposal. The desired wheel diameter, load and use life are specified. The model then determines the alloy content, forging strain and final wheel thickness that minimize the life cycle cost.

The use and disposal costs for the wheel can be reduced by decreasing the thickness of the wheel. This can be achieved by increasing the strength of the material. This, in turn, can be achieved either by increasing the alloy content or by increasing the cold work. The first method increases the raw material and disposal costs. The second increases the manufacturing costs. The question

is: what alloy composition, casting geometry and wheel thickness minimizes the total cost of material, manufacture, use and disposal? Cold forging is assumed for the sake of simplicity.

The diameter thickness, strength and cost all evolve during manufacture, but in the present model only cost continues to evolve during use. A more sophisticated model could be envisaged where strength continues to evolve during use due to such phenomena as recovery, fatigue and corrosion.

There are three steps in the analysis: (i) There is an overall cost scaling that depends on the volume, V, of the disc. This volume, in turn, depends on the material strength, as influenced by the alloy content and the strain hardening introduced by cold forging. (ii) Another cost factor relates to the work done in cold forging, W, which governs the energy consumption. (iii) A formula must be found that combines all of the life cycle costs, which may be differentiated to find the *minimum.*

The volume of material, which is conserved during forging is

$$V = (\pi/4)d_o^2 h_o = (\pi/4)d_1^2 h_1 \tag{3.1}$$

where the subscript o refers to the cast state and 1 refers to the forged state. The strains introduced by forging harden the material. The appropriate relationships are given by standard results from deformation processing. The effect of strain ε on material strength S is given by

$$S = S_o\left[1-\exp(-A\varepsilon)\right], \tag{3.2}$$

the strain ε is related to the thickness reduction by

$$\varepsilon = \ell n(h/h_o), \tag{3.3}$$

the initial strength S_o is related to the alloy content a_o by

$$S_o = S^*(1+Ba_o) \tag{3.4}$$

with A, S^* and B being well-known material constants. The condition for meeting the load requirement is

$$S_1 h_1 = D \tag{3.5}$$

where D is coefficient determined from the diameter and elastic constants of the wheel and the design load. Combining the above results, the volume V becomes

$$V = \frac{\pi d_1^2 D}{4S^*(1+Ba_o)\left[1-\exp(-A\varepsilon_1)\right]} \tag{3.6}$$

This formula provides one scale factor for the cost analysis.

The work of forging per unit volume of material is

$$\begin{aligned} W &= \int_o^{\varepsilon_1} S\,d\varepsilon \\ &\equiv S^*(1-Ba_o)\left\{\varepsilon_1 - \left[1-\exp(-A\varepsilon_1)\right]/A\right\} \end{aligned} \tag{3.7}$$

This is another scaling factor.

The life cycle cost C_L is now specified as

$$C_L/V = \alpha(1+\beta a_o) + \gamma w_1 + \delta + \phi(1+\mu a_o^2) \tag{3.8}$$

where the first term is the cost of the casting; the second, the cost of manufacture; the third, the cost of operation; and the fourth, the cost of disposal. The coefficients α, β, γ, δ, ϕ and μ are cost factors. Combining the above formulae gives

$$C_L = \frac{\pi d_1^2 D}{4S^*(1+Ba_o)\left(1-e^{-A\varepsilon_1}\right)}\left[\alpha+\delta+\phi+a\beta a_o+\phi\mu a_o^2+\frac{\gamma S^*(1+Ba_o)}{A}\left(A\varepsilon_1-1+e^{-A\varepsilon_1}\right)\right] \tag{3.9}$$

This gives the life cycle cost, C_L, as a function of the two variables: casting alloy fraction, a_o, and forging strain, ε_1.

The minimum life costs can be obtained by taking the partial derivatives of Eqn. (3.9) with respect to a_o and ε_1 and setting them equal to zero. This gives,

$$e^{A\varepsilon_1} - 1 - A\varepsilon_1 = \frac{A\left(\alpha + \delta + \phi + \alpha\beta a_o + \phi\mu a_o^2\right)}{\gamma S^*\left(1 + Ba_o\right)} \tag{3.10}$$

and

$$Ba_o^2 + 2a_o + \frac{\left[\beta\alpha - B\left(\alpha + \delta + \phi\right)\right]}{\phi\mu} = 0 \tag{3.11}$$

Equation (3.11) can be solved to obtain the optimum value of composition, a_o. Then, Eqn. (3.10) can be solved to obtain the optimum value of forging strain, ε_1. Finally, the optimum value of forging thickness can be obtained as

$$h_1 = \frac{D}{S^*\left(1 + Ba_o\right)\left(1 - e^{-A\varepsilon_1}\right)} \tag{3.12}$$

This basic approach of combining physical principles with cost parameters could clearly be broadened to many other products, materials and processes.

4. STATUS OF PROCESS MODELS

4.1 General Factors

A report has recently been compiled in the U.K. by Sargent, Shercliff and Wood regarding materials processing technologies. Many of the issues raised have their counterparts in the U.S. The essential conclusions are used here.

1. General Process Modelling

Much process model development is conducted in the context of a narrow processing area, and does not lead to general results. A methodology which extracts generic modelling methods from many processes is preferable. An additional issue is the selection of appropriate modelling

techniques for the problem (both technically and economically). Both goals require a systematic means of classifying modelling problems in terms of the process physics and solution techniques.

2. Classification of Modelling Problems

Conventional classifications by process type provide limited guidance. As an example: friction-welding has more to do with *forging* than gas-metal-arc welding. In building process models, it is useful to follow this sequence:

- Identify the classes of physical phenomena within the process to be modelled.
- Identify the mathematical equations which describe the relevant physics.
- Using the parameters in the equations as a guide, identify data needs: (a) material properties and constitutive laws, (b) boundary conditions, and (c) eventual validation of the model.

Further considerations in model construction relate to software structure, choice of appropriate algorithm, etc. These have a bearing on all of the above stages.

From the point of view of process model development, more useful classifications may be based on: (i) the physical process involved, (ii) the coupling between these processes, (iii) the differential equations which describe each process, (iv) the boundary conditions of the system, (v) the nature and availability of materials data. This generic view places all issues concerned with materials science, computational power, parameter measurement, software modularity, model usability, etc., in a single context. [Computing power cannot compensate for poorly understood physics.]

Classification by Physics

It should be possible to identify the occurrence and importance of physical phenomena within the process to be modelled: convection, radiation, conduction, elastic deformation, small plastic deformations, large plastic deformations, diffusion, chemical reactions, magnetic fields, acoustic energy transmission, etc. Identification of the *time constants* and *length scales* controlling the underlying physics is also important in decoupling multi-physics behavior, and in determining if

a mechanism can be treated as operating in a continuum manner, or if its spatial distribution must be modelled explicitly. This approach also assists in deciding when it is appropriate to transfer modelling techniques between superficially similar materials. [Methods developed for steel cannot uniformly be applied to aluminum alloys.]

Classification by Coupling

Identifying the direction and strength of coupling between physical processes guides the choice of boundary conditions and for constructing algorithms. For example, some hot working processes have partly decoupled temperature and deformation fields - the temperature strongly affects the strain field, but not vice versa. Hence the temperature field can be evaluated first using an "average" strain, and then be superimposed on a more detailed deformation calculation.

Classification by Differential Equations

Process models invariably involve description in terms of sets of ODEs or PDEs, which may be elliptic, hyperbolic or parabolic equations; dependent on time, spatial dimensions, field variables and internal states. Each type of PDE/ODE formulation coupled with particular types of boundary conditions and mesh-type can be "best" solved by a different algorithm; where "best" involves robustness, accuracy and speed. These considerations also indicate when to use analytic algebraic equations and when to construct a discrete meshed model. There are only four reasons for using a meshed method:

- the modelled volume has some complex shape
- the modelled volume contains numerous internal structures (e.g. grains)
- the modelled volume contains discontinuous behavior
- the underlying process physics are non-linear

Complexity of shape is a subtle issue. Geometric complexity may not imply complexity in physical phenomena (diffusion, heat flow, etc.) Assumptions such as "semi-infinite" in a given problem may also prove to be valid for some materials and not for others.

Classification by Boundary Conditions

Boundary conditions (BCs) form another classification system (Dirichlet, Cauchy, or Neumann type). The most appropriate solution techniques depend rather critically on the exact types of

PDEs, BCs and the types of coupling between the different PDEs. Determining the boundary conditions of a problem is a major part of the activity of process modelling.

3. Influence of Physical Data

In all models there is a need for numerical values of material property and boundary condition parameters. Data always comes at a cost, often very high, and this must be included in an overall evaluation of the costing of the whole modelling activity. Experiments needed to validate a model should also be planned and costed as far as possible before the model is constructed. Making approximations in the data (e.g. neglecting temperature-dependence) is also a business decision, since this influences the cost, accuracy and value of the information emerging from the model. Difficulties with data for boundary conditions are dominated by heat transfer coefficients and friction behavior. Two complicating conditions relating to data can occur which impede industrial transfer of process models: (a) if the measurements required are prohibitively expensive or laborious; (b) if the data are capricious, in that measurements are extremely sensitive to variations from one sample to another (notably surface properties).

Sensitivity Analysis

Sensitivity analysis of any model, with respect to variation in the values of the materials parameters is always necessary. The qualitative behavior of the model with respect to parametric variation is often of much more use than the simple numeric "answer" produced by the model when "fed" the best estimates of the materials parameters. Studying the sensitivity of a model to variations in one material parameter at a time is a common, but limited, method. In general, a Taguchi-style matrix of sensitivity is required, due to the inherent nonlinearity of the behavior.

4. Goals and Costs of Process Modelling

Process models are predominantly driven by commercial needs, rather than by general fundamental scientific endeavor. The goals of such models usually fall within the following list:

- to develop a new or scaled-up process
- to reduce iteration in trials (better speed and cost)
- to optimize an existing process to reduce cost
- to improve quality and yield by reducing product and process variability
- to provide model-based process control

The industrial context and purpose of the process modelling task strongly constrains the modelling methods. Simple models based on a few first order effects can produce significant savings from just getting an improved first "guess". More complex models are needed if the issue that must be understood is the result of second order effects. Improving quality by reducing variability nearly always requires second order effects to be taken into consideration leading to more complex models. This also requires a greater range and detail of experimental data to provide parameters and validation tests. "Reduced modelling" of complex (slow) process models is desirable to make the results more widely available, and applicable to problem solving where the level of detail is not as great as in the most difficult case.

In general, refining a simple model with more complex physics is a matter of diminishing returns. Doubling the complexity, with exponential rises in modelling cost, leads to much less than double the benefit in having the model. It is worth noting that once a useful model is implemented, any refinement is likely to add cost at no added benefit until the model can make a significant step forward.

The usefulness of a model can only be seen in comparison with other ways of estimating the same information. Models are not necessarily cheaper or faster than performing a real experiment. The asymmetry in information between simulation and experiment is, however, significant. For example, a well-instrumented casting is more expensive than a simple trial, but a model can display results with "virtual" thermocouples everywhere.

As far as the cost of modelling a processing operation is concerned, there is wide agreement that it is dominated by manpower of analysis and programming (80%), excluding the cost of acquiring materials parameter values. (These costs can be very high if measured from a fully functioning plant which would otherwise be producing products.) Szekely estimated a total cost of $120,000 for a reasonably complex model taking one man-year to develop. The range was from $20-30,000 for a "simple exercise" to many millions for a "really complex model". Hardware for process modelling is apparently not an issue. Costs are dominated by salaries, software and support.

The type of technology/company is an important factor in evaluating the relative costs and benefits of modelling. In large high technology companies, resources are more likely to be available to support more expensively trained and experienced modellers, to set up experiments to provide data. Since greater benefits in terms of profits and reduced lead-times are likely,

additional modelling costs can be justified more readily. However, from a national perspective, the modelling needs of small to medium, lower technology companies should not be neglected.

4.2 Solidification

The modelling of solidification processes is a difficult task for two reasons: firstly, the presence of a liquid phase makes it necessary to consider mass and species transport and secondly, this process involves a phase transition having a large latent heat release (i.e., strong, non-linear effects). Furthermore, the solute and thermal diffusion length scales being widely different in metallic alloys (typically a factor 10^4), the solidification microstructure which develops upon cooling of the melt is much smaller than the scale of the process. Considering the calculational power to today's computers, it is therefore *not yet possible* to model a solidification process with the spatial resolution of the microstructure.

Major efforts have been made over the past thirty years to simulate the complex phenomena intervening in solidification processes. Most of them have been directed towards the macroscopic scale (i.e., the scale of the process). For that purpose, the continuity equations governing the exchange of heat, mass and solute within the solidifying domain are averaged over the liquid and solid phases, assuming local equilibrium at the scale of the microstructure. These equations resume to the standard continuity equations in the pure liquid/solid phases but new terms appear for the mushy zone (i.e., the zone where the fine microstructure develops). In particular, these terms account for the latent heat release and the segregation of solute species, which are associated with the phase transformation. The momentum conservation equation is equivalent to the Navier-stokes equation in the liquid phase but a Darcy-type term, which is a function of the local volume fraction of solid, is added in order to model interdendritic fluid flow in the mushy zone.

Two- and three-dimensional Finite Element (FEM) or Finite Difference (FDM) codes, which solve the average continuity equations for complex geometries, now exist on the market. Even the mould filling stage, for which the free liquid surface must be taken into account, can be modeled. The information which can be obtained from such macroscopic models (temperature, velocity and solute fields) is very useful for optimizing a given process and to minimize the macroscopic defects (cold shuts, isolated pockets of liquid leading to macropores, macrosegregation, freckles, etc.). Combined with recent solidification theories, such information allows determination of some of the parameters of the microstructure (dendrite arm/trunk spacing, eutectic spacing, etc.). Criteria functions based on the thermal gradient, the growth rate and the cooling rate have also be derived in order to predict the grain morphology and, in

particular, the transition between columnar and equiaxed grains (i.e., between grains nucleated at the surface and in the bulk of the liquid, respectively). similar functions have been used for the prediction of defects, such as microporosity or stray crystal formation. Although very useful to the practitioner, such criteria functions are empirically based and often lack a sound physical background.

More recently, the average continuity equations governing the transport phenomena at the macroscopic scale have been coupled with microscopic models describing the heterogeneous nucleation, growth and impingement of grains. Even though such micro-macroscopic models ignore the effects associated with convection, they allow determination of the final grain size and phase repartitioning. Originally based upon a deterministic approach, these models have now been implemented using probabilistic methods, such as the Monte Carlo (MC) or Cellular Automata (CA) techniques. Such methods can account for the random location and crystallographic orientation of new nuclei, which form either in the bulk of the liquid or at the surface of the casting, for the growth kinetics of the microstructure and for the preferential growth directions of dendrites. Coupled with FEM and FDM heat flow calculations at the macroscopic scale of the process, probabilistic modelling directly produces computed micrographs. It can thus predict the morphology of the grains and their impingement, the columnar-to-equiaxed transition, the growth competition of the grains near a re-entrant corner or in the grain selector of a turbine blade, etc. The evolution of the crystallographic texture of the grains which occurs in the columnar zone of a casting can also be simulated using such methods.

At present, the micro-macroscopic modelling of solidification of multicomponent alloys is mainly based upon simplified phase diagrams. An effort is being made to couple the continuity equations of solute species with the calculation of complex phase diagrams as obtained, for example, from Thermocalc™. Microsegregation models are also refined in order to encompass out-of-equilibrium effects at the local scale (e.g., partial solute diffusion in the solid).

A remaining challenge concerns the complex issue of predicting various macroscopic defects that arise from stresses and displacements, such as hot tearing and residual-stress-induced cracking. To meet this challenge, the community involved in solidification modelling must collaborate with the applied mechanics and structural materials groups familiar with non-linear stress analysis, creep rupture and cracking. The formation of such a linkage represents one of the objectives of the proposed effort.

4.3 Welding

The state of welding modelling is quite heterogeneous. Certain common processes, such as arc welding, have been studied in enough detail that empirical weld models exist which offer recommended welding parameters for a set of standardized weld geometries and methods. Even here, subtle effects such as the Marangoni effect can nullify the predictions. In this example, small variations in impurities can change the temperature dependence of the surface tension from positive to negative, with a corresponding change in the circulation pattern in the weld pool. Such changes in fluid circulation patterns can drastically alter the penetration depth. Other welding processes are even less well characterized, because the physics is difficult. Keyhole welding processes, such as electron beam welding and laser welding, in particular, are notoriously difficult to model because of the multiple competing physical processes. In electron beam welding, the heat input from the beam is influenced by metal vaporization, electromagnetic effects, fluid flow and heat flow. Building a process model that takes into account all the applicable physics would result in a code that *would severely tax computing resources.* Attempts are being made to model the slightly simpler case of laser welding, for which electromagnetic effects are less critical. Even here, combining the effects of fluid flow, solidification, heat flow and metal vaporization stretch the current modelling capabilities. Such models represent a great scientific challenge for applied physics and materials science.

5. COST ESTIMATION

Process selection for the manufacture of a component or structure with mechanical functions is commonly based on expertise or on established local practice. What is needed is a systematic approach which identifies, from the large range of processes available, the sub-set capable of making a given component or structure from a given material, to a given shape and with a given precision or finish. This can partly be done by considering the attributes of processes themselves. But, in the end, it is the cheapest process route that we seek. A cost-based procedure for selecting processes should be developed which runs as background to any modelling activity. It can be based on a summation of material costs, tooling (capital) cost and labor (time-dependent) costs modified by factors which depend on design features. The aim should be to develop a flexible methodology, exploiting readily available information, which might guide the selection and development of processes at early stages in the design.

Life cycle models of the type illustrated above would be the most complete and would have the greatest eventual impact. Yet, there are still major opportunities for cost models that address

some aspects of the life cycle. Particular progress has been made on models for costing generic manufacturing methods. These are based on a global approach which gives a breakdown of contributions from the material, capital expenditure and various rate dependent phenomena.

Manufacturing cost estimation methods exist at several levels ranging from macro to micro. Macro models develop relationships between a cost ratio R and total batch weight, with R being the ratio of product cost C_p to material cost, C_m. A formula for R is

$$R = 1 + \frac{C_c}{wnC_m} + \frac{\dot{C}_t}{w\dot{n}C_m} \tag{5.1}$$

C_c = capital cost (time-independent)
$\dot{C}_t$ = labor cost rate (time-dependent)
n = number of units
w = mass of unit

such that

wn = total tonnage
$w\dot{n}$ = rate of production

The functional relationship for R is plotted on Fig. 5.1. Processes evolve to optimize R by either increasing the production rate, $w\dot{n}$, or decreasing the labor cost rate C_t. The postulate used for further analysis is

$$\dot{C}_t / w\dot{n} \sim 1/C_c^m \tag{5.2}$$

where m is a power law coefficient. Upon using this proportionality with Eqn. (5.1), a minimum in R with respect to C_c exists. This minimum defines the optimum process envelope, designated R_{opt}. It is given by (Fig. 5.2)

$$R_{opt} = 1 + \frac{(R_o - 1)}{(wn)^{m/(m+1)}} \tag{5.3}$$

This result establishes the influence of batch size on the cost ratio, through the initial value, R_o.

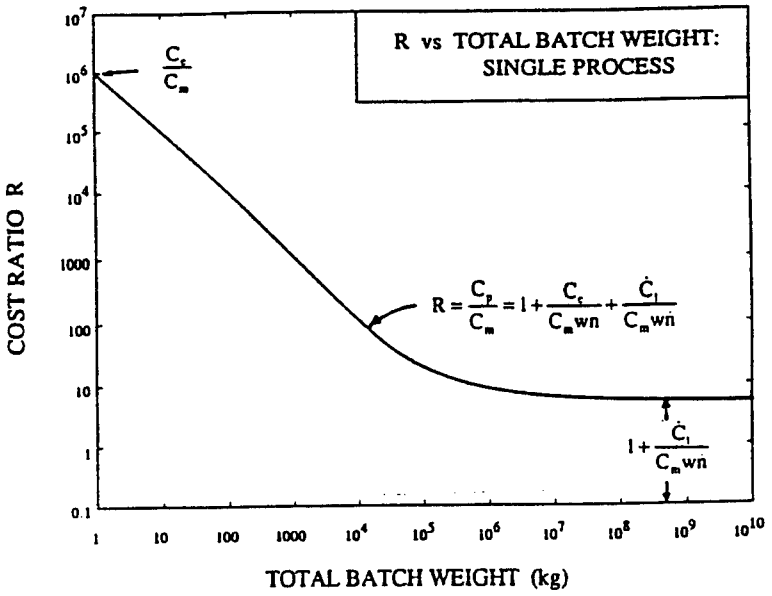


Figure 5.1

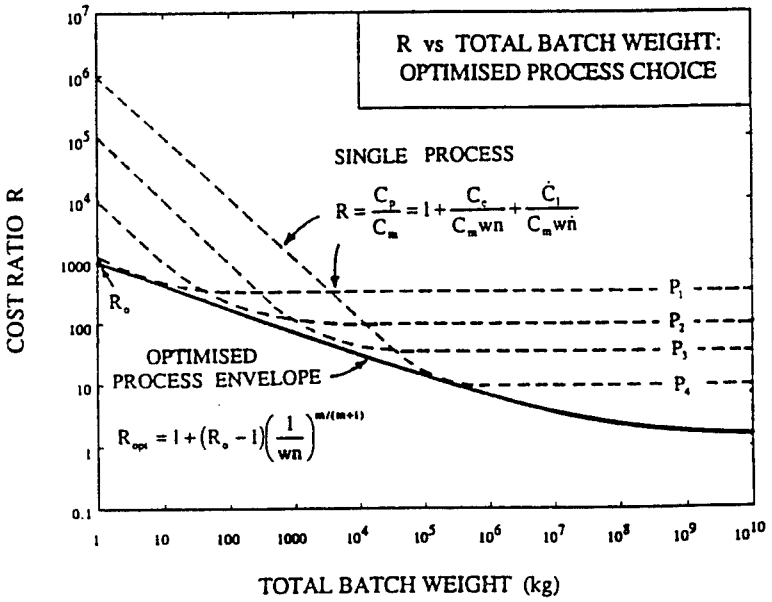


Figure 5.2

The capital and labor costs are based on known processes, but scaled using a mesomodel to allow for changes in the size, shape and complexity of the product, as well as changes in precision required in the process, as sketched on Fig. 5.3.

An example relevant to the production of glass fiber-reinforced plastic (GFRP) by two processes (Fig. 5.4)—one manual and one automated—illustrates the roles of the different variables. In this case, the material cost C_m has two contributions: one from the fiber and the other for the matrix.

The time-dependent variable $\dot{C}_t$ is governed largely by the time to process a part, t_p. It should include energy costs, as well as actual labor costs. The capital costs C_c include the number of machines and tools, as well as the building. However, there are dependencies of capital costs on process time, via the number of production lines.

Evaluation of the time t_p is amenable to theoretical approaches. For example, in injection moulding, the cooling time t_c in the mould is important. This time can be determined analytically as

$$t_c = \frac{\rho d^2 C_p}{\pi^2 k} \ell n\left[\frac{8}{\pi^2}\frac{(T_{melt} - T_{tool})}{(T_{eject} - T_{tool})}\right] \tag{5.4}$$

with C_p being the specific heat, ρ the density, d the part dimension and k the thermal conductivity. There is an additional contribution to the cycle time associated with mould filling, which depends on the part weight.

6. PRODUCT PERFORMANCE AND PROPERTY PROFILES

The attributes of a product are fundamentally related to composition, microstructure and defects, through a property profile. A spectrum of models exists which attempt to relate specific physical properties to the microstructure and composition. Also in existence are formulae that relate design criteria to property combinations, through merit indices. These are available in a software format through the Cambridge Materials Selector. In combination, these models and formulae relate design to microstructure, composition and defects. Corresponding life analysis models which relate fatigue, corrosion, etc. to microstructure and composition are sparse and

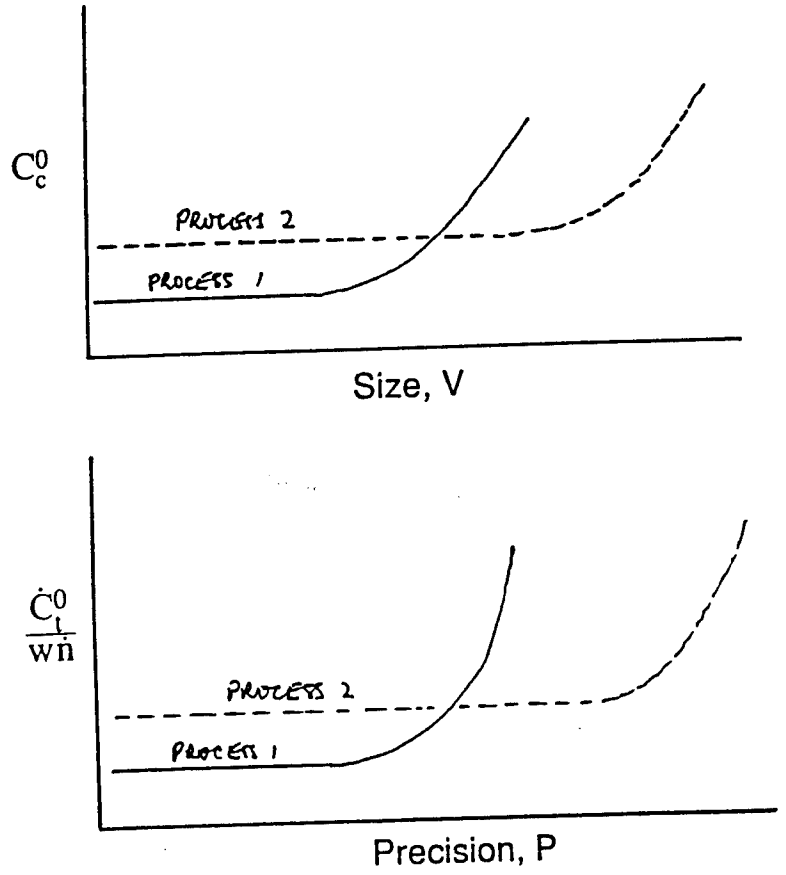

C_c^0
PROCESS 2
PROCESS 1
Size, V
$\frac{\dot{C}_L^0}{\dot{w}n}$
PROCESS 2
PROCESS 1
Precision, P

Figure 5.3

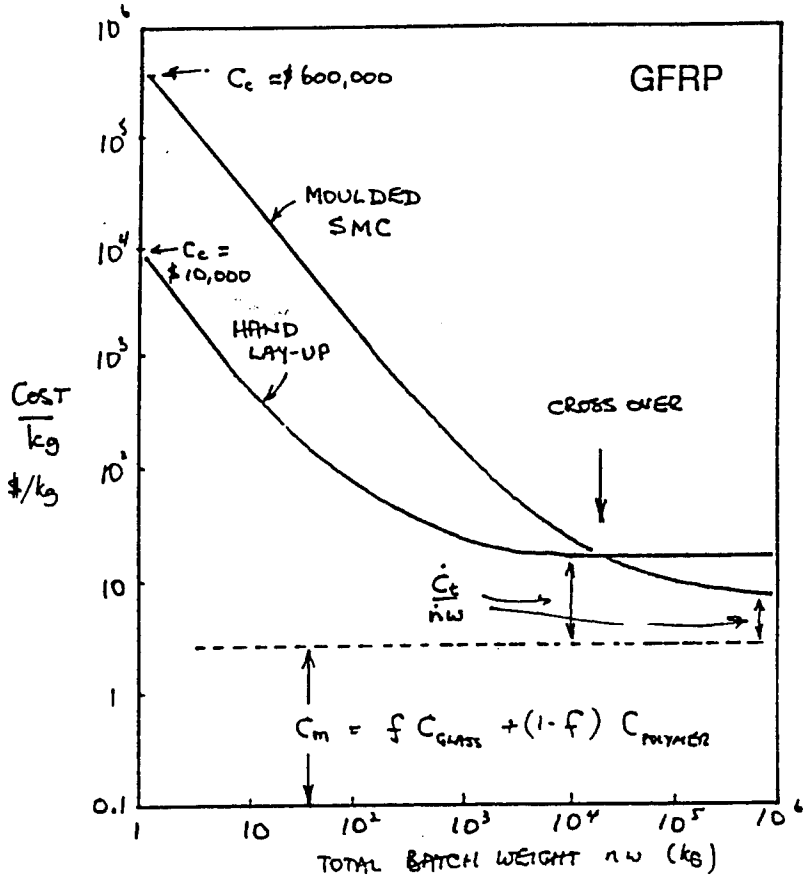

GFRP
C_t = £600,000
MOULDED SMC
C_t = £10,000
HAND LAY-UP
CROSS OVER
$\frac{\dot{C}_t}{nw}$
$C_m = f\,C_{GLASS} + (1-f)\,C_{POLYMER}$
COST / kg
£/kg
TOTAL BATCH WEIGHT nw (kg)
10^6
10^5
10^4
10^3
10^2
10
1
0.1
1
10
10^2
10^3
10^4
10^5
10^6

Figure 5.4

underdeveloped. Most corrosion models, for example, have had a focus on understanding rather than life prediction.

A synopsis is given of models that relate to product performance, compatible with a state variable concept, as well as an accompanying bibliography. The intent of this synopsis is to illustrate the philosophy and status of models that can be readily integrated with process models that contain microstructural information. It also attempts to highlight deficiencies in property models which would need to be addressed for the eventual success of the proposed strategy. It is rarely possible to predict properties by having knowledge only of the microstructure. However, in many cases, the property models identify the relevant microstructural parameters and their non-dimensional groupings. In such cases, the properties can be characterized over a wide range by conducting a relatively few experiments to determine the coefficients and the exponents. Examples are given in the following.

Some thermophysical properties can be evaluated through fundamental atomistic level calculations. These include elastic properties and thermal expansion coefficients. This capability is expected to have considerable importance for the Knowledge Highway because, often, the data base for such fundamental properties is sparse. The intention would be to interact with software programs now under development (e.g., at Biosym) that would calculate such properties. Some illustrations are given below.

i) Atomistic Level Codes

Various atomistic methods are available which allow various properties of materials to be calculated. These will soon be available in software programs, being developed by Biosym and others. Atomistic simulation allows the user to determine the structure and energy of ensembles of atoms. If this ensemble consists of a defect in an otherwise perfect crystal, atomistic simulations can determine both the structure of the defect and the defect energy. Atomistic simulations can also be used to determine the vibrational properties of solids, coefficient of thermal expansion, the Gruneissen constant, etc.

All atomistic simulations require a description of the atomic interactions; i.e., the energy of the system as a function of the arrangement of its atoms. Several methods are available to determine these energetics. These include, in order of decreasing rigor, *ab initio,* quantum mechanics based methods, semi-empirical, quantum mechanics based methods and physically based empirical methods. The advantage of the *ab initio* methods is that they are generally reliable since they accurately solve for the electronic structure of the material. These methods include FLAPW,

FLMTO, pseudo-potential based method and several atomic cluster based methods. Although several *ab initio*, quantum mechanics based electronic structure methods have been used in atomistic simulations, they generally require very extensive computational resources and hence may only be practically employed with static relaxation methods. Semi-empirical quantum mechanics based descriptions of the energetics, such as the tight-binding method also are based upon electronic band structure methods, but are parameterized in terms of empirical functions often fit to *ab initio* results. The use of tight binding methods is becoming an increasingly popular and highly successful method for atomistic simulations of covalently bonded materials, such as Si. The tight binding theory has also been successfully applied to describe metallic alloys. The least reliable, but generally most computationally efficient description of the energetics is based upon physically motivated, empirical interatomic potentials. These include such well-known potentials as the Lennard-Jones potential for ideal gases, the Embedded Atom method (EAM) and Finnis-Sinclair potentials for metals, the Stillinger-Weber and Tersoff potentials for Si and the Buckingham and shell models for ceramic materials.

In choosing the appropriate description of the atomic interactions, there is a trade-off between computational efficiency and reliability. Therefore, the atomistic simulation routines are being written with sufficient generality that any of these schemes could be used. Furthermore, since several new classes of potentials are under development, the atomistic simulation codes would accommodate new classes of interatomic potentials.

The atomistic simulation tools would include:

- Static Relaxation
- Monte Carlo (MC)
- Molecular dynamics (MD)

All of these methods may be applied to finite clusters of atoms with arbitrary applied stress. The static relaxation method is based upon the minimization of the energy of the system with respect to the positions of all of the atoms. Since this method does not account for entropy, it may only be directly applied at zero temperature. However, the static relaxation method can be used to map out an energy surface which, when combined with classical transition state theory, can be employed to calculate reliable finite temperature properties. The static relaxation method is the most computationally efficient of the three methods listed above for determining equilibrium structures.

Both the Monte Carlo and Molecular Dynamics methods may be applied at finite temperature. The MC method (in its most commonly used form) accounts for the entropy of the system by randomly sampling different atomic configurations according to Boltzmann statistics. MD is based upon integrating Newton's equations of motion for each atom—where the force is evaluated from the energy of the system. In MD, the entropy is included in the form of the thermal motion (vibration) of the individual atoms. Typical integration time steps in MD are generally no greater than a tenth of an atomic vibrational time period (i.e., ~ 10^{-15} seconds in metals) and hence, MD can only be used to efficiently sample fast events. MC simulations, on the other hand, provide no dynamical information, but do provide a more efficient sampling of the configurational phase space of the system.

A new hybrid simulation technique, based upon the efficient, static relaxation method, extends this method to finite temperatures and the grand canonical ensemble. This approach is based upon the minimization of an approximate free energy functional with respect to atomic positions and concentration profiles. Aside from efficiency, the main advantage of this method over MC and MD is that it provides a simple, approximate method for determining the free energy and all thermodynamic properties of solid alloys.

ii) Elastic Properties

Elastic properties (bulk and shear modulus, Poisson's ratio) can be modelled at two levels: atomistic and continuum. The atomistic models can be used to predict single crystal elastic properties. The quantum mechanical methods required for this purpose can still be computationally restrictive, particularly when non-cubic crystal structures are involved and when solid solutions occur. Here, it is important to note that the less computationally intensive, approximate atomistic methods (such as the embedded atom method (EAM)), are *incapable* of predicting elastic properties. Instead, they use these properties to calibrate the interatomic potentials for calculating other properties, such as surface energies. Some recent progress has been made using the Linear Muffin Tin orbital method. This area will continue to develop without additional motivation.

Continuum models are available for predicting the elastic properties of two phase (or multiphase) materials, based on the properties of the constituents. These 'composite' models give elastic properties that depend on volume fraction, distribution and shape, but must be independent of size. Results have been obtained using cell models and lattice spring models, as well as by self consistent and differential self consistent methods. These models provide useful upper and lower bounds. However, the models are only useful if the constituent elastic properties are *known* and

that the morphology and distribution of the phases, including the porosity, have been quite accurately predicted by the process models. This requirement provides specific objectives for the process models.

Unbonded interfaces and microcracks are problematic because such features can substantially diminish the effective moduli. Their influence on elastic properties can be calculated, but their incidence is difficult to predict. Such incidence is known to depend on size, as well as the morphology and the thermal expansion mismatch. With this knowledge, it may be possible to develop rules capable of estimating these effects.

iii) Flow Strength

Dislocation models have been developed for a wide range of plastic flow phenomena. In principle, these models relate the flow strength to microstructure. However, they have not been widely used to correlate variations in strength with explicit microstructural changes. In many cases, this can be done by appreciating the attributes and limitations of the models. Generally, the dislocation models can be expressed in the form of non-dimensional groups with quite well-defined magnitudes of the exponents. However, the coefficients are not predicted with adequate precision. Nevertheless, the coefficients can be calibrated by means of a small number of carefully chosen experiments and then used to predict the behavior over a wide range. The approach is illustrated below for precipitation hardened Al alloys.

In precipitation hardened alloys, there are contributions to the strength from alloy elements in solution and from the precipitates. The latter depends on whether the precipitates are shearable or non-shearable.

The contribution to strength from solid solution elements, $\Delta\sigma_s$, is related to their concentration $\bar{c}$ and can be represented by the non-dimensional parameter (NDP),

$$\Delta\sigma_s/G\bar{c}^{2/3} = \lambda_1 \tag{6.1}$$

where G is the shear modulus and λ_1 is an unknown coefficient.

The contribution from precipitates susceptible to shear, $\Delta\sigma_{ps}$, is related to their volume fraction f and radius R by,

$$\Delta\sigma_{ps}/G\sqrt{fR/b} = \lambda_2 \tag{6.2}$$

where b is the Burgers vector. For precipitates that resist shearing and are bypassed, the contribution to strength $\Delta\sigma_{pb}$ is

$$\Delta\sigma_{pb}/Gb\sqrt{f} = \lambda_3 \tag{6.3}$$

The relative incidence of precipitate shearing and by-pass is governed by the particle size distribution, with a smooth transition. Moreover, these mechanisms *compete,* such that the one giving the lower strength dominates. The overall precipitate strengthening is thus represented by the harmonic mean,

$$\Delta\sigma_p = \left[1/\Delta\sigma_{ps} + 1/\Delta\sigma_{pb}\right]^{-1} \tag{6.4}$$

The NDP is

$$\frac{\Delta\sigma_p}{G}\sqrt{\frac{fR}{b}} = \frac{1}{\lambda_2} + \frac{1}{\lambda_3}\left(\frac{R}{b}\right)^{3/2} \tag{6.5}$$

The final expression for the strength is the sum, $\Delta\sigma_s + \Delta\sigma_p$.

A process model capable of predicting the yield strength would need to contain information about the shear modulus, G, the volume fraction and size of the precipitates and the concentration of the solution. It is also required that some experiments be done to calibrate λ_1, λ_2 and λ_3. The procedures are described in the paper by Shercliff and Ashby.

For duplex microstructures and composites, the situation is less satisfactory. While models exist, there are some unresolved issues. One issue relates to fine scale plasticity and strain gradient effects. These are manifest as a transition in the formulae that relate flow strength to microstructure. Size *independent* behavior occurs at large length scales ($\gtrsim$ 1μm). Such behavior can be simulated using laws of continuum plasticity. However, size dependent behavior arises at smaller length scales, which must be modelled by using dislocation mechanics. Recent progress in this area is encouraging, but incomplete.

Physically based models (Johnson-Cook, Zerilli-Armstrong) for flow strength that account for temperature, strain rate and strain hardening already exist in code and are readily available in

some of the standard FEM and hydrodynamics codes, such as ABAQUS, EPIC, DYNA, NIKE, MESA. The range of validity for each model varies widely, depending on the data set used to fit the parameters of the model. Also, texture in polycrystalline materials can now be accounted for in a fully quantitative manner, although the material models are more expensive to use in a FEM context. The Highway would take advantage of these existing capabilities and help define the limits of their capabilities.

iv) Fracture Resistance

The fracture resistance of a material is a straightforward concept. It is related to the inelastic mechanisms that operate, as a crack extends. It is governed by the energy dissipated per unit area of new crack surface. Expressed in terms of a fracture energy, Γ, the cracking resistance is the product of the stress at which the inelastic mechanism operates, designated σ_o, and the dimension normal to the crack plane within which dissipation occurs, designated b. At the simplest level, the non-dimensional parameter (NDP) that governs fracture is

$$\Sigma = \Gamma/\sigma_o b \tag{6.6}$$

The magnitude of Σ at which the crack grows is dependent on the *mechanism* of crack growth. Some examples are given below. The proposed focus on an integrated methodology would require that σ_o and b be identified for each fracture mechanism and moreover, that both quantities be related to microstructural features that emerge from process models.

A particularly useful output of fracture studies would be fracture mechanism maps, building onto basic concepts developed earlier by Ashby and colleagues. There are two fundamentally different modes of fracture: brittle and ductile. Additional mechanisms operate at high temperature under creep conditions. A parameter that clearly and unambiguously separates ductile and brittle behavior (based on crack tip mechanisms) has yet to be devised. However, recent progress has been considerable and identification of such a parameter can be expected. In the interim, an empirical classification scheme can be used.

While ductile fracture is expected to occur in accordance with a single mechanism, there are many mechanisms that can arise in materials subject to brittle fracture. At this stage, it is not possible to predict the mechanism that dominates by only having knowledge of the microstructure. A classification scheme is needed to identify the most likely dissipation mechanism. Then, in some cases, interpolations can be made which *predict* the influence of small changes in microstructure. Three examples illustrate the present status.

In materials that exhibit a *ductile fracture* mechanism, the hole coalescence phenomenon that causes cracks to extend is well-known. But still, the energy expended upon initial crack growth, Γ_o, cannot be predicted based only on knowledge of the microstructure. Cracks extend by the growth and coalescence of small holes that form ahead of the crack, by a plastic flow process operating in the stress field of the crack. The fracture energy is thus controlled entirely by plastic dissipation. The stress quantity entering the NDP, Σ is the plastic flow strength, σ_p, and the dimension is the spacing between holes, ℓ

$$\Sigma_1 = \Gamma_o/\sigma_p\ell \tag{6.7}$$

However, this information is not sufficient. In most practical, structural materials, the holes form at the hard particles used for strengthening (as well as at inclusions). The incidence of holes at these particles and inclusions is not predictable. Qualitatively, hole formation is known to depend on particle size and morphology and upon the interface with the alloy matrix. While appreciable thought has been given to this phenomenon in alloy design programs, research essentially stopped before reaching the goal of relating Γ_o to microstructure. Nevertheless, enough of the mechanics is known that it might be feasible to establish meaningful microstructural objectives within specific categories of structural alloy.

In metals that fail by *cleavage,* fracture originates by the formation of microcracks in hard particles near the crack front. Crack growth occurs when the elastic/plastic stress field around the crack is sufficiently large to cause the microcrack formed in the particle to extend dynamically into the metal. In this case, the particle size R is the relevant length scale and the yield strength, σ_o, is the critical stress. However, the phenomenon is statistical in nature and other terms enter the NDP. Moreover, the resistance of the matrix to dynamic crack growth is also important, manifest in the magnitude of its fracture energy, γ_p. The consequent NDP is

$$\Sigma_2 = \frac{\Gamma_o \sqrt{f\,d}\,\sigma_o^{N-1} R^{(N-2)/2}}{E^{(N-1)/2}\,\gamma_p^{(N+1)/2}} \tag{6.8}$$

where N is the work hardening coefficient and d is the grain diameter, which determines the spacing between the particles. In this case, the NDP is well-represented by constituent properties that relate to microstructure. Moreover, it is possible to predict the transition from cleavage to ductile fracture, by equating Σ_d and Σ_c. The potential for an integrated approach appears to be promising.

In dual phase materials that derive their toughness from a ductile phase, the crack growth resistance Γ_s is dominated by plastic dissipation occurring in the ductile phase. This happens within a zone dictated by the *diameter,* 2R, of this phase, which becomes the length scale. The critical stress is again the flow strength, σ_o. The NDP is,

$$\Sigma_3 \equiv \Gamma_s/Rf\sigma_o \tag{6.9}$$

where f is the volume fraction of ductile phase. Again, the microstructural information contained in the NDP suggests an opportunity for an integrated approach.

v) Fatigue

There are no quantitative models that predict fatigue life, knowing the microstructure. The yield stress is often used as a threshold suitable for design. In such cases, the preceding yield models would be relevant. When crack growth contributes to the fatigue life, the crack growth rate may usually be characterized by a Paris Law, determined by experiment. There are relatively small effects of microstructure on crack growth (within any specific alloy system). However, fatigue life can be strongly influenced by inclusions and porosity, which enhance crack nucleation. Adequate crack nucleation models have yet to be devised.

8. MATERIAL PROPERTIES FOR MODELLING AND SIMULATION

8.1 Data Bases

Access to the material data needed for modelling is typically a limiting factor. It is of major importance that the Knowledge Highway be linked to the Data Bases that exist and are under development. The present situation is briefly reviewed, through two sources. One is a review by Kaufman and Drago. The other concerns an effort under development at the Cambridge University Design Center (CUDC).

The former describes two networks: the Material Property Data Network (MPD) and the Chemical Property Data Network (CPD). The primary need is single-point access to a wide variety of reliable numeric (quantitative) material performance and application data. The preferred source is that with the greatest combination of breadth and depth. The next important need is ease of access. Difficulties in accessing a source may be sufficient to cause the search to

be abandoned. The relative motivation for system use depends upon the relative simplicity, clarity and flexibility of the search software for the candidate systems.

To be of value, a data source must provide:

- a critical mass of numeric data; a high probability of useful answers;
- ease of access; a 'quick connection';
- flexible search and retrieval software; multiple search paths;
- strong system support; integrated thesaurus, help functions;
- capabilities for handling and downloading the data.

These are the objectives behind the development of the CPD and MPD Networks. These are referred to as 'networked' because, within each, the databases are networked physically by the search software and intellectually by the search strategies and the associated thesauri, which cross-link the terminology in the various databases. These are truly network services within the context of the broader scientific and technical network and permit concurrent searching of all of the databases networked in each cluster, regardless of the service centers the individual databases reside on.

Numeric property data have characteristics not shared by more conventional bibliographic data. They are quantitative and thus have implied precision, come in ranges, as well as discrete values and may vary over many orders of magnitude within a single data record containing four or five properties. Second, they have units associated with them from which they can never be separated. The numbers in any one record may have multiple units. Finally, they are usually dependent upon a number of independent variables or combinations of variables (designated parameters) which influence their value.

Numeric data must be stored and searched, keeping in mind at least three major elements—the name of the property, its value and the units of that value—and often more. For example, the property may be dependent upon time of exposure at a particular combination of temperature and pressure and so three more factors—time, temperature and pressure—must be included as delimiters in every query about that property.

The CPD services include such classes of properties as thermodynamic, electrochemical, spectral, safety and transport. Among the specific databases currently available through the prototype version are:

DIPPR—textual and numeric information on the pure component physical property data for commercially important chemical substances;
HODOC—an electronic version of much of the CRC Handbook of Data on Organic compounds, including the chemical and physical properties of over 25,000 organic substances;
JANAF—critically evaluated thermodynamic properties from the Joint Army-Navy-Air Force Thermodynamic Tables;
NISTTHERMO (formerly NBSTHERMO)—the NIST Tables of Chemical Thermodynamic Properties, containing critically evaluated chemical thermodynamic properties of over 8000 inorganic and organic substances;
NISTFLUIDS (formerly NBSFLUIDS)—the NIST calculation package covering the thermophysical and transport properties of fluids as a function of temperature and pressure;
TRCTHERMO—from the Thermodynamic Research Center—the evaluated thermodynamic properties of 7000 compounds.

In addition, the CPD service makes significant use of the NUMERIGUIDE database to identify properties and to locate the databases that will likely contain the data the user desires. NUMERIGUIDE is a property thesaurus and data directory that provides:

- property names and hierarchies,
- definitions/descriptions,
- aliases,
- abbreviations,
- identification of databases that address each property,
- default units, and
- variables associated with property (e.g., temperature).

Numeric information available on the MPD service includes not only mechanical, physical and other performance data for all structural materials, including metals, polymers, ceramics and composites, but also the properties of connections and joints in these materials. Among the specific databases available through the MPD service are:

AASD—from the Aluminum Association—typical and minimum tensile properties, typical mechanical and physical properties and fabricating and application information on more than 150 commercial alloys;
ALFRAC—from NIST/SRD, the Materials Properties council and the aluminum Association—plane strain fracture toughness data for about 25 high-strength aluminum alloys, with validity documentation;

COPPERDATA—from the Copper Data Association—mechanical, electrical, thermal and other physical properties of wrought and cast US copper and copper alloys;
IPS (International Plastics Selector)—from DATA Business communications, a division of IHS;
MIL-HDBK-5—from the MIL-HDBK-5 Coordination committee publication—design tables covering the design mechanical and physical properties of ferrous and non-ferrous alloys;
MARTUF—from the Materials Property Council—abut 10,000 individual toughness test results for steels for marine applications;
METALS DATAFILE—from Materials Information (ASM International and the Institute of metals)—data from more than 40,000 literature citations from technical journals;
MPDSEARCH—an international directory of sources for material property information that contains both databases and data centers—organizations who will research information for you;
NISTCERAM—from NIST—properties of structural ceramics—silicon carbides and silicon nitrides;
PDLCOM—from the Plastics Design Library—chemical and environmental compatibility of plastics;
PLASNEWS—a daily news file for the plastics industry;
PLASPEC—from the publishers of Plastics Technology—typical properties from producers of about 10,000 plastics; and
STEELTUF—from the electric Power Research Institute and the Materials Properties Council—results of more than 20,000 individual tests of steels for the power and petroleum industries.

All the features listed below are available on the CPD and MPD services.

- range searching—the ability to search for chemicals or materials with combinations of properties in specific ranges or above or below certain limiting values;
- unit conversion—the ability to convert to any of the worldwide standard systems of units—International Standard (SI), meter-kilogram-second (MKS), centimeter-gram-second (CGS), engineering (ENG) and the STN user-friendly SI system;
- tolerance setting—the ability to define ranges of search values by the tolerance on the search value (e.g., 5,000 ± 1000 psi);
- table display—the ability to obtain tabular display of data that match your specific query and to predefine certain types of tabular displays; and

- calculation packages—the capability for interpolation and estimation of additional information or the application of parametric analysis of multi-variant properties, valuable in providing specific answers to some complex materials questions.

To best service the needs of searchers for properties data, many databases have been linked together into a logical 'cluster.' Depending upon the nature of a query, CPD and MPD service users approach the database cluster with different pieces of information at the heart of their query:

- a specific database with a certain type of data, e.g., design values;
- a specific chemical or material for which a variety of types of data are sought;
- a specific property or properties for which a comparison of chemicals or materials is required, perhaps involving a specific range of values, notably those equaling or exceeding certain limiting values.

The CPD and MPD services enable the user to search all of the databases in the cluster simultaneously, with no requirement that the user know which databases are most likely to contain the data. Further, from such a cluster, all reasonable data sets responsive to the query are provided, always with clear evidence of why they were provided and from where they have come along with all of the associated parametric support data. In the case where answers to the same query are located in two or more different databases, the user is always given the option of selecting individual answers or comparing all of them; no analysis is made, but rather the user may decide which to use based upon the relative merits of the replicate values.

8.2 Property Checking and Estimation

The properties of solids have values which - for a given structure and bond-type (defining a "class" of solid) - lie within broadly defined ranges, characteristic of the class. Beyond this, correlations exist between values of mechanical, thermal, electrical and other properties which derive from the underlying physics of the material and can be expressed as dimensionless groups with much narrower value-ranges. These allow a physically-based consistency check on property values, and allow some properties to be estimated when values for others are known. The ability to do this is useful whenever calculations involving material properties are undertaken. The correlation suggests sensible normalizations for property groups which appear in physical modelling, and they help identify classes of material to which a given model might apply. The ranges and correlations allow the detection of errors in the values of data; and they permit calculations to proceed even when some data are missing by providing intelligent estimates for the missing values. It is practical to develop software to provide automatic data checking and (when necessary) estimation as a module which could be interfaced with any one of numerous

modelling activities. It complements the procedures for computing properties from first principles.

9. PRODUCT-ORIENTED METHODOLOGY

9.1 Diffuser Cases For Propulsion Units

9.1.1 Background

Diffuser cases are critical, high-temperature, pressure vessel components within a propulsion unit. They are modular in nature (Fig. 9.1) and made from Ni-based superalloys. They can be manufactured either by casting or by a combination of casting, forging and welding. The components must resist creep deformation and have good thermomechanical fatigue (TMF) resistance. Presently, diffuser cases are made from IN 718. This material is not the preferred choice from a design perspective because it has relatively low creep and fatigue strength. It is used for its manufacturability: particularly its weldability. The potential for simultaneously optimizing the material, the process and the cost in order to achieve performance objectives, by means of an integrated modelling approach is thus an attractive scenario for this component.

The basic idea would be to choose IN 718, plus a material with superior creep/fatigue characteristics, and to link models that examine products made either by casting or by welding. The emphasis would be on a typical sub-element for the overall diffuser case, such as that indicated on Fig. 9.2. This sub-element has all of the key features found in a case, but still has sufficient geometric simplicity to allow creep/fatigue testing.

Process/microstructure models for casting and for welding will be implemented and new features added to the models by additional research. The intended outcome would be models that predict the microstructure, macrosegregation in casting, residual stresses and macrodefects such as hot tears, macroporosity and cracks.

Existing creep/fatigue models for superalloys will be implemented and again, additional features will be added through further research. The intent would be to have models of creep deformation, creep rupture and TMF that connect directly to the microstructural and defect information generated from the process/microstructure models.

Each stage of the process and performance models generates scaling factors that can be introduced into a life cycle cost model. This model would be developed by starting with the Cambridge University Software and adding new features.

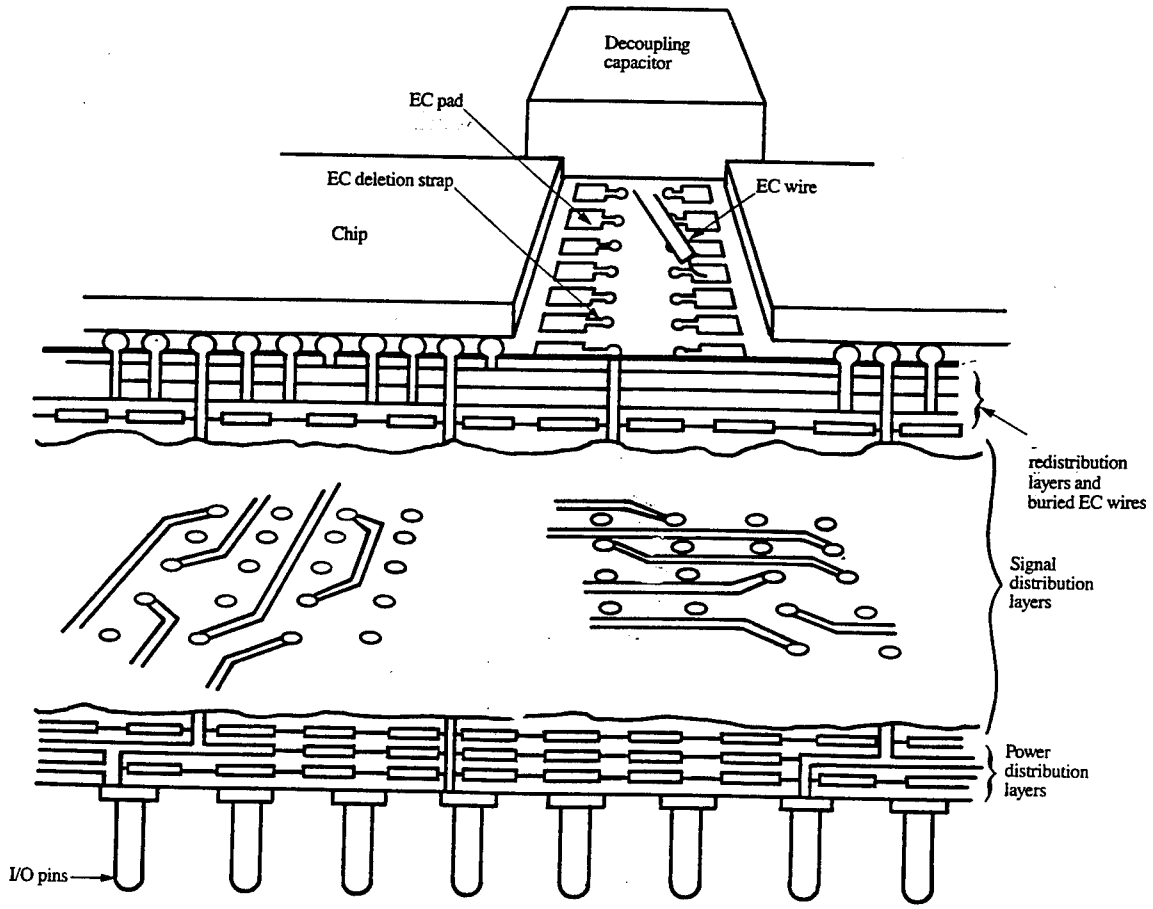
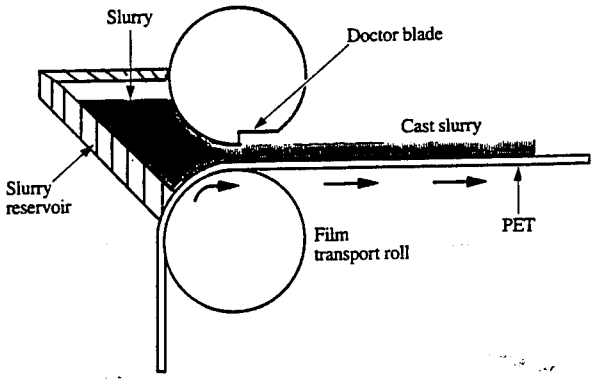
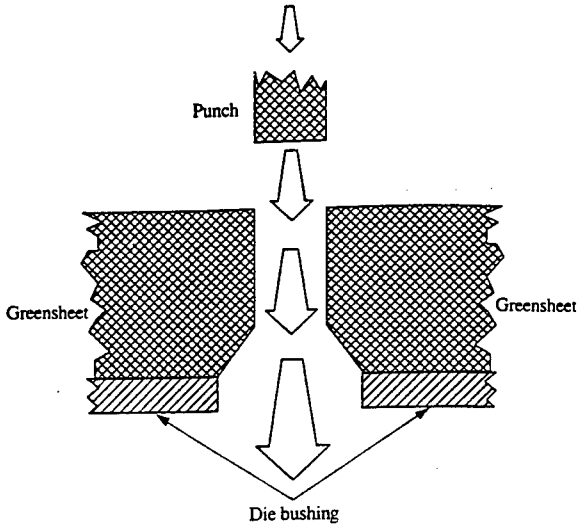

Decoupling capacitor
EC pad
EC deletion strap
Chip
EC wire
redistribution layers and buried EC wires
Signal distribution layers
Power distribution layers
I/O pins

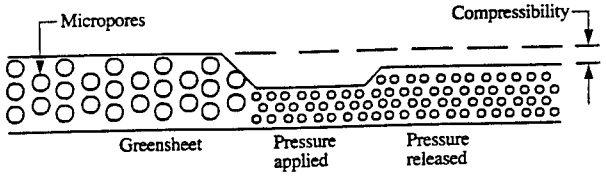
Figure 9.1

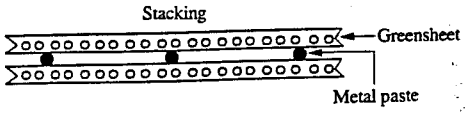


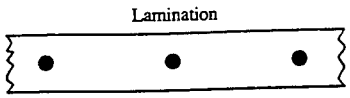
Doctor blade and casting assembly.



. greensheet punching.







Greensheet compressibility and metal line enclosure at lamination.

Figure 9.2